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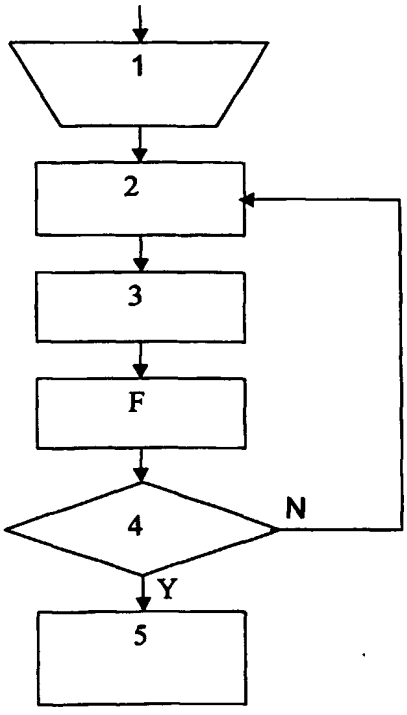
(54) Title: SAMPLING METHOD



(57) **Abstract:** The present invention is an incremental umbrella sampling method to improve the performance of established sampling methods. It is sampling the state space by iteratively generating states $_{xi,t}$ and their weighting factors represented by Formula (a) by fitting the sampling distribution function $p_f(x)$ of the next iteration to at least one weighted property of the already sampled states. This means that $p_f(x)$ is fitted to the product represented by Formula (b), in which Formula (a) is the weighting factor and $O(_{x,i})$ is a function respectively a property of the states $x_{i,t}$. The number of states $x_{i,t}$ and the number of weighting factors (see Formula (a)) is incremented with each iteration. In order to have a consistent set of weighting factors (see Formula (a)), the weighting factors are recalculated in each iteration for all, respectively for a set of selected, states. By fitting $p_f(x)$ in the state space it is possible to use all the information of Formula (a) and $O(x_{i,t})$ for the states $x_{i,t}$ generated so far. The fitting step allows to use different fitting strategies. For example the fitting can bias the sampling away from areas where intensive sampling has been done in the preceding iterations, or the sampling can be directed along local gradients respectively towards local minima or maxima of one or several weighted properties. In each of the iterations, the sampling distribution function is fitted in a way to improve the overall sampling of the state space. The method supports multi-objective optimisations. State space integrals can be solved. It reduces the probability that the system is trapped. The invention is general. It can be used with different sampling methods, in particular with Monte Carlo sampling, Metropolis Monte Carlo sampling, or dynamic simulations. It can be combined with the concepts of simulated annealing and multicanonical sampling. It provides a general framework that can be adapted to the system and the observables of interest.

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